

AD-A111 815

MAINE UNIV ORONO DEPT OF PHYSICS AND ASTRONOMY

F/G 20/13

PHASE DIAGRAM OF ISING MODELS WITH RANDOM SUBLATTICE VACANCIES.(U)

FEB 82 C HU, P KLEBAN

N00014-79-C-0441

NL

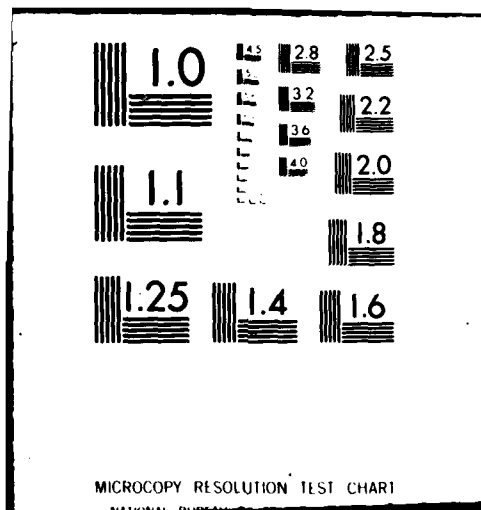
UNCLASSIFIED

TR-7

1-1  
2-1



END  
DATE  
FILMED  
4-82  
DTIC



ADA111815

DTIC FILE COPY

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE (5)		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER Technical Report #7	2. GOVT ACCESSION NO. ADA111 815	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) Phase Diagram of Ising Models With Random Sublattice Vacancies		5. TYPE OF REPORT & PERIOD COVERED Technical Report
		6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) Chin-Kun Hu and Peter Kleban		8. CONTRACT OR GRANT NUMBER(s) Contract #N00014-79-C-0441
9. PERFORMING ORGANIZATION NAME AND ADDRESS Department of Physics and Astronomy University of Maine Orono, Maine 04469		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS Project #NR392-032
11. CONTROLLING OFFICE NAME AND ADDRESS Office of Naval Research Physics Program Office Arlington, VA 22217		12. REPORT DATE February 1982
		13. NUMBER OF PAGES 13
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)		15. SECURITY CLASS. (of this report) unclassified
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE
16. DISTRIBUTION STATEMENT (of this Report)  Approved for public release; distribution unlimited		
17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)		
18. SUPPLEMENTARY NOTES Submitted to Physical Review		
19. KEY WORDS (Continue on reverse side if necessary and identify by block number) Ising model with random vacancies, square lattice, body centered cubic lattice, transition temperature, modified Kadanoff's variational method, linear decrease of transition temperature, percolation, critical proba- bilities for percolation		
20. ABSTRACT (Continue on reverse side if necessary and identify by block number)  See first paragraph		

DD FORM 1473  
1 JAN 73

EDITION OF 1 NOV 65 IS OBSOLETE  
S/N 0102-014-6601

DTIC  
SELECTED  
MAR 9 1982  
H

PHASE DIAGRAM OF ISING MODELS WITH  
RANDOM SUBLATTICE VACANCIES

Chin-Kun Hu and P. Kleban

Department of Physics and Astronomy

and

Laboratory for Surface Science and Technology

University of Maine  
Orono, Maine 04469, USA

Abstract

We use a modified Kadanoff's variational method to calculate the phase diagram of an Ising model with random vacancies on one of two interpenetrating sublattices of the isotropic square (SQ) and body-centered cubic (BCC) lattices. We find second order phase transitions only for  $T > 0$ . The transition temperature to very good approximation decreases linearly with impurity (i.e. vacancy) concentration at small concentration. This agrees with the linear decrease observed in other systems. A plausible explanation of the absence of first order transitions for  $T > 0$  is given.

The relation of our models to certain percolation problems is similar to that of some spin models studied by Syozi. Thus our results allow an estimate of critical probabilities for percolation.

1. Introduction

In recent years, much attention has been paid to extensions of the ordinary spin 1/2 Ising model, such as the Potts model<sup>1-3</sup> and spin one models<sup>4-11</sup>. An example of the latter is the Blume-Capel model<sup>4,5</sup> represented by the Hamiltonian:

$$H = -J \sum_{\langle nn \rangle} S_i S_j - D \sum_i (1 - S_i^2) - B \sum_i S_i \quad (1)$$

where  $s_i, s_j = 1, 0, -1$ ,  $\sum_{\langle nn \rangle}$  is a sum over nearest neighbor  $s_i, s_j$  on the lattice, and  $D$  is the zero-field splitting parameter. Eq. (1) may be considered as an Ising

model with annealed impurities (or random vacancies) represented by the zero component of spins  $s_i$ . The thermal average impurity concentration is controlled by the parameter  $D$ . As  $D/J \rightarrow \infty$ , the system reduces to the pure Ising model. Mean field<sup>5-6</sup>, Monte-Carlo<sup>8</sup>, and renormalization group<sup>9-11</sup> (R G) studies of Eq. (1) indicate that the order-disorder phase transitions of this model consist of a line which is first order at low temperatures and second order at high temperatures. It is generally agreed that two regions meet at a tricritical point; however, the location of this point is not exactly known.

In this paper, we apply a modified Kadanoff's Variational method (MKVM)<sup>12-15</sup> to calculate the phase diagram of a related model given by:

$$H = -J \sum_{\langle nn \rangle} \sigma_i s_j - D \sum_j (1 - s_j^2) - B \sum_i \sigma_i - B \sum_j s_j, \quad (2)$$

where  $\sigma_i = \pm 1$ ,  $s_j = 1, 0, -1$ ,  $\langle nn \rangle$  denotes nearest neighbors as in Eq. (1),  $J > 0$  and  $D$  is a zero-field splitting parameter for  $s_j$ . We consider Eq. (2) for SQ and BCC lattices in two and three dimensions respectively. We give results for the  $B=0$  case only. The spins  $s_j$  are located on one of two interpenetrating sublattices, the spins  $\sigma_i$  on the other. The two dimensional case is illustrated in Fig. 1. In three dimensions the spins  $\sigma_i$  sit on a simple cubic lattice with a spin  $s_j$  at the center of each unit cell. Eq (2) may be considered as an Ising model with annealed impurities or vacancies present on any site  $j$  of one sublattice when  $s_j = 0$ . The thermal average of impurities is controlled by  $D$  as in Eq. (1). As  $D/J \rightarrow \infty$ , Eq (2) also reduces to a pure Ising model. In sect. II, we calculate phase diagrams of our model and find that the order-disorder transitions of Eq (2) for  $T > 0$  consist of a line of second order transitions only. The first order line found in the phase boundary calculated from Eq. (1) is no longer present. A plausible argument for this difference is given. In sect. III, we consider our models at  $T \rightarrow 0$ . Our models are closely related to some systems studied by Syozi<sup>16</sup>. Each of these spin models has a corresponding percolation problem. The spin system phase boundary for the order-disorder transition at  $T \rightarrow 0$  gives an accurate estimate of the critical probability for the corresponding percolation problem. Thus, the critical percolation

probabilities for our models may be estimated from our calculated phase boundaries at  $T \rightarrow 0$ .

## II. Method of Calculation and Results

The method of calculation is essentially the same as that reported in previous papers<sup>13-14</sup>. We briefly review it here. We consider Eq (2) for two dimensional square (SQ) and three dimensional body-centered cubic (BCC) lattices. The Hamiltonian of Eq (2) may be rewritten as:

$$H = -\sum_R V_R, \quad (3)$$

$$V_R = JS_R (\sigma_1 + \dots + \sigma_z) + D (1 - S_R^2) + \frac{B}{z} (\sigma_1 + \dots + \sigma_z) + BS_R, \quad (4)$$

where  $R$  is a unit hypercube of the  $\sigma$  spin lattice with  $z (=2^d, d$  being the space dimension)  $\sigma$  spins at the corners and one  $s$  spin in the center. This is illustrated in Fig. 1 for the two dimensional case. Performing an exact decimation calculation for the partition function of Eq. (3), which sums over the central  $s$  spin in each cell, we obtain an effective Hamiltonian for the remaining  $\sigma$  spins. The resulting unit cell potential is:

$$V_{\text{eff}} = \beta B (\sigma_1 + \dots + \sigma_z) / z + \beta D + \ln \{ 1 + 2 \exp (-\beta D) \cosh (\beta B + \beta J (\sigma_1 + \dots + \sigma_z)) \}, \quad (5)$$

where  $\beta = \frac{1}{kT}$ . In two dimensions, for the case  $B = 0$ , which we examine below, Eq (5) is equivalent to a  $\sigma$  spin Hamiltonian with nearest neighbor, next nearest neighbor, and four spins (around a unit hypercube) interactions. In three dimensions, there are also six and eight spin interactions. For given  $J, D$  and  $\beta$ , we then use Eq (5) as  $\tilde{V}_0$ , the initial cell potential, and carry out the step by step RG transformation. We calculate the free energy ( $f$ ), internal energy ( $U$ ) and spontaneous magnetization ( $M$ ) per spin (here  $M \propto \langle \sigma_i \rangle + \langle s_j \rangle$ ). The average occupation number of the zero component of  $s$  spin  $\langle n_0 \rangle$ , ie the concentration of impurities or vacancies, is given by:

$$\langle n_0 \rangle = - \frac{\partial f}{\partial (\beta D)} = \frac{1}{2} \langle 1 - s_i^2 \rangle \quad (6)$$



Accession No.	RTIS GRAAL	Transmitted	Justification	By	Distribution/Availability	Dist
DTIC TAB						

$\langle n_0 \rangle$  is calculated using the chain rule, by the same method used to calculate  $U$  and  $M$  (Eq (17) of paper 14 with  $q$  representing  $\mu D$ ). As  $D/J \rightarrow -\infty$  or  $\infty$ ,  $\langle n_0 \rangle \rightarrow 0$  or  $0.5$  respectively. From the behavior of the coupling constants (tending to larger or smaller values), we know whether the system is in an ordered or disordered state. From a simple ground state energy argument, it is obvious that for  $B = 0$  the order-disorder transitions occur only in the region  $\frac{D}{JZ} \leq 1$ . The MKVM<sup>14-15</sup> is known to give accurate values for the transition temperature over a wide range of parameter values.

The calculated phase diagrams (for  $B = 0$ ) are shown in Fig. 2, where  $T_0$  is the transition temperature of the pure Ising model calculated with the MKVM method, which gives  $\frac{J}{kT_0} = 0.4576223$  and  $0.1621341$  for the SQ and BCC lattices respectively. For comparison, the exact<sup>17</sup> or series expansion<sup>18</sup> values of  $\frac{J}{kT_0}$  for SQ and BCC lattices are  $0.44068679\dots$  and  $0.15740 \pm 0.0003$  respectively. The part of the diagram under the curve is in an ordered state and above the curve in a disordered state. We calculated  $U$ ,  $M$  and  $\langle n_0 \rangle$  near the phase boundary and found that there is no discontinuity across the phase boundary even as  $\frac{D}{JZ} \rightarrow 1$  and  $T_c \rightarrow 0$ . For example, for SQ lattices at  $\frac{D}{JZ} = 0.9925$ , we found that  $\Delta U \approx 10^{-16}J$ ,  $\Delta \langle n_0 \rangle \approx 10^{-13}$  and  $\Delta M \approx 10^{-2}$  where  $\Delta Q \equiv Q(T+\epsilon) - Q(T_c-\epsilon)$  with  $Q$  being  $U$ ,  $\langle n_0 \rangle$  or  $M$ ,  $T_c$  being the phase transition temperature for given  $\frac{D}{JZ}$  and  $\epsilon$  being a very small number. The  $\Delta Q$  values just mentioned are of the same order of magnitude as numerical errors arising from truncation and the approximate location of  $T_c$ , etc. We may thus conclude that the transition is always second order rather than first order for  $T > 0$ . In Fig. 3, we have converted the phase diagram of Fig. 2 to  $T_c/T_0$  versus  $\langle n_0 \rangle$ . It is interesting to note that as  $\langle n_0 \rangle$  approaches the critical concentration  $\langle n_0 \rangle_c$ , above which there is no phase transition at all,  $T_c$  decreases smoothly to zero at  $\langle n_0 \rangle_c = 0.26$  in the SQ lattice while  $T_c$  jumps rapidly to zero near  $\langle n_0 \rangle_c = 0.42$  in the BCC lattice. In the later case  $U$  and  $M$  still change continuously when crossing the phase boundary. Mean field<sup>6</sup> and Monte-Carlo<sup>8</sup> studies of the phase diagram for the Blume-Capel Model (on a SQ lattice) indicate that at  $T = 0$ ,  $\langle n_0 \rangle_c$  for this model is 1.0.

The part of Fig. 3 for small  $\langle n_0 \rangle$  is enlarged and reproduced in Fig. 4, which indicates that, to very good approximation,  $T_c$  decreases linearly with  $\langle n_0 \rangle$  for small  $\langle n_0 \rangle$ . The slopes of the straight lines in Fig. 4 are  $1.683 \pm 0.002$  and  $1.116 \pm 0.001$  for SQ and BCC lattices, respectively. The phase transition temperatures of the Ising model with quenched<sup>19</sup> or annealed<sup>20</sup> bond impurities have also been studied by series expansion method and are found to decrease linearly with small impurity concentration. It has also been observed experimentally<sup>21</sup> that in nickel-rich, nickel-titanium alloys the ferromagnetic Curie temperature decreases, to very good approximation, linearly with titanium concentration  $x$ , for  $x \leq 1.5\%$ . The approximately linear decrease of  $T_c$  with small impurity concentration is perhaps a rather general phenomena.

Now, we give a plausible explanation for the absence of a first order phase transition in the model of Eq. (2) for  $T > 0$ . A system at a second order phase transition is characterized by an infinite correlation length  $\xi$ , ie a perturbation at one point can propagate to points an infinite distance away. In the model of Eq. (2), the impurities (zero component of  $s_j$ ) appear only on one sublattice. In the region of interest,  $\frac{D}{JZ} < 1$ , the spins  $\sigma$  on the other sublattice always have non-zero effective coupling (see Eq. (5)). Thus the correlation length can easily extend to infinity at  $T_c$ , in contrast to the model of Eq. (1), where impurities can appear in both sublattices and thus more easily destroy the propagation of a perturbation from one point to another far away point.

We can also understand the absence of first order transitions as follows. For a square lattice one expects a first order transition for  $\frac{D}{4J} \lesssim 1$ , at low  $T$  values, if it exists anywhere. It follows from Eq. (5) that the (exact) decimation of the spins  $s_i$  generates (for  $B = 0$ ) effective nearest neighbor, next nearest neighbor, and four spin interactions that we denote  $J_{nn}$ ,  $J_{nnn}$ , and  $J_4$  respectively. By permutation symmetry one has  $J_{nn} = J_{nnn}$ . In general,  $J_{nn} > 0$  for ferromagnetic  $J$  ( $J > 0$ ). In the region of possible first order transitions one can show that  $J_4 > 0$  as well. Thus when the vacancies are summed away all interactions promote



ferromagnetic ordering of the  $\sigma$  spins in this region, and a second order transition (of simple Ising type) is to be expected, as we find in our MKVM calculation. The conclusion of the absence of first order transitions on a BCC lattice for  $\frac{D}{8J} < 1$  can also be reached by a similar argument.

### III. Low Temperature Limits

Syozi<sup>16</sup> has calculated the exact phase diagrams of Ising models on decorated square (SQ), honeycomb (HC) and <sup>plane</sup> triangular (PT) lattices with spins  $s = \frac{1}{2}$  on each lattice site and spins  $s = 1$  on each nearest neighbor bond. He also calculated phase diagrams for Ising models on <sup>a</sup>semi-dilute honeycomb lattice: where the spins  $s = \frac{1}{2}$  and  $s = 1$  spins are on two equivalent interpenetrating sublattices as in the present case. The phase boundaries of Syozi's models at  $T \rightarrow 0$  give the critical concentration  $P_c$  of spins ( $1 - P_c$  is the vacancy concentration) on sites of  $s = 1$  spins above which ferromagnetism can occur. It turns out that  $P_c$  calculated in this way is exactly equal or very close to the critical probability of the corresponding bond<sup>22</sup> (for decorated lattices) or sublattice-site (for <sup>a</sup>semi-dilute HC lattice) percolation problems. For the Syozi model:

$$P_c (\text{decorated SQ}) = 0.5$$

$$P_c (\text{decorated PT}) = 1 - P_c (\text{decorated HC}) = \frac{5(3-\sqrt{3})}{18} = 0.3522 \dots$$

$$P_c (\text{semi-dilute HC}) = 0.5.$$

For the percolation problem 22, 23.

$$P_c (\text{bond, SQ}) = 0.5$$

$$P_c (\text{bond, PT}) = 1 - P_c (\text{bond, HC}) = 2 \sin \frac{11}{18} = 0.349 \dots$$

$$P_c (\text{sublattice site, HC}) = 0.5 \quad (8)$$

It is obvious that our model of Eq (2) on the SQ and BCC lattices is just an Ising model on a semi-dilute SQ or BCC lattice and its low temperature behavior is similar to the Syozi models. Thus, the critical probabilities  $P_c$  of the sublattice-site percolation problem on the SQ and BCC lattices can be estimated from  $\langle n_0 \rangle_c$  of Fig. 3.  $P_c$  is given by :

$$P_c = 1 - 2 \langle n_0 \rangle_c. \quad (9)$$

Applying Eq. (9) to  $\langle n_0 \rangle_c$  of Fig. 3, we have  $P_c = 0.48, 0.16$  for the SQ and BCC lattices respectively.

#### Acknowledgments

The authors are indebted to Professor R. B. Griffiths for useful discussion and the referee for valuable comments on our paper. This work was supported by the Office of Naval Research.

### Figure Captions

- Fig. 1. Lattice of Eq. (2) in two dimensions. Dots (.) spins  $\sigma_i$ , crosses (x) spins  $s_j$ . The dotted lines enclose a unit hypercube of the  $\sigma$  spin lattice.
- Fig. 2. Transition temperature  $T_c$  vs.  $D/Jz$  obtained for a two dimensional SQ (+) lattice and a three dimensional BCC ( $\Delta$ ) lattice.
- Fig. 3. Transition temperature vs. impurity concentration  $\langle n_0 \rangle$  for a SQ (+) and a BCC ( $\Delta$ ) lattice.
- Fig. 4. Part of the curves in Fig. 3 for  $\langle n_0 \rangle < 2.6\%$ . The solid curves are obtained by a linear least square fit to the data points.

# References

1. R. B. Potts, Proc. Cambridge Philos. Soc. 48, 106 (1952).
2. B. Nienhuis, A. N. Berker, E. K. Riedel and M. Schick, Phys. Rev. Lett. 43, 737 (1979).
3. B. Nienhuis, E. K. Riedel and M. Schick, J. Phys. A 13 L31 (1980).
4. M. Blume, Phys. Rev. 141, 517 (1966).
5. H. W. Capel, Physica (Utr.) 32, 966 (1966); 33, 295 (1967); 67, 423 (1967).
6. M. Blume, V. J. Emery, and R. B. Griffiths, Phys. Rev. A4, 1071 (1971).
7. R. B. Griffiths, Physica 33, 689 (1967).
8. B. L. Arora and D. P. Landau in Magnetism and Magnetic material -1972 (Denver) edited by C. D. Graham and J. Rhyne, AIP Conf. Proc. 10, 870 (1973).
9. A. N. Berker and M. Wortis, Phys. Rev. B 14, 4946 (1976).
10. T. W. Burkhardt, Phys. Rev. B 14, 1196 (1976).  
T. W. Burkhardt and H. J. Knops, Phys. Rev. B 15, 1602 (1977).
11. M. Kaufman, R. B. Griffiths, J. M. Yeomans and M. Fisher, Phys. Rev. B 23, 3448 (1980).
12. Y. M. Shih, et.al., Phys. Rev. B 19, 529 (1979).
13. C. K. Hu, et.al., Proc. of the National Science Council, Taiwan, Roc 4, 359 (1980).
14. C. K. Hu and P. Kleban, (to appear in J. Comp. Phys.)
15. C. K. Hu and P. Kleban submitted to Phys. Rev. B.
16. I. Syozi, Prog. Theor. Phys. Japan, 34, 189 (1965); I. Syozi and S. Miyazima, Prog. Theor. Phys. Japan, 36, 1083 (1966); J. W. Essam and H. Garelick, Proc. Phys. Soc. 92, 136 (1969).
17. L. Onsager, Phys. Rev. 65, 117 (1944).
18. M. F. Sykes, D. L. Hunter, D. S. McKenzie, and B. R. Heap, J. Phys. A 5, 667 (1972).
19. A. B. Harris, J. Phys. C 7, 1671 (1974).
20. D. C. Rapaport, J. Phys. C 5, 1830 (1972).
21. Y. K. Yao, S. Araj and K. U. Rao, Chin. J. Phys. (Taipei) 15, 1 (1977).
22. J. W. Essam in Phase Transitions and critical phenomena, edited by C. Domb and M. Green (Academic, London, 1972) Vol.2, P 197.
23. In the sublattice-site percolation problem, the sites on one of two equivalent sublattices are occupied completely by atoms (ie with probability 1), the sites of the other sublattice are occupied with probability P. The sublattice-site percolation problem on a honeycomb lattice is equivalent to the site percolation problem on a triangular lattice where critical probability is 0.5.

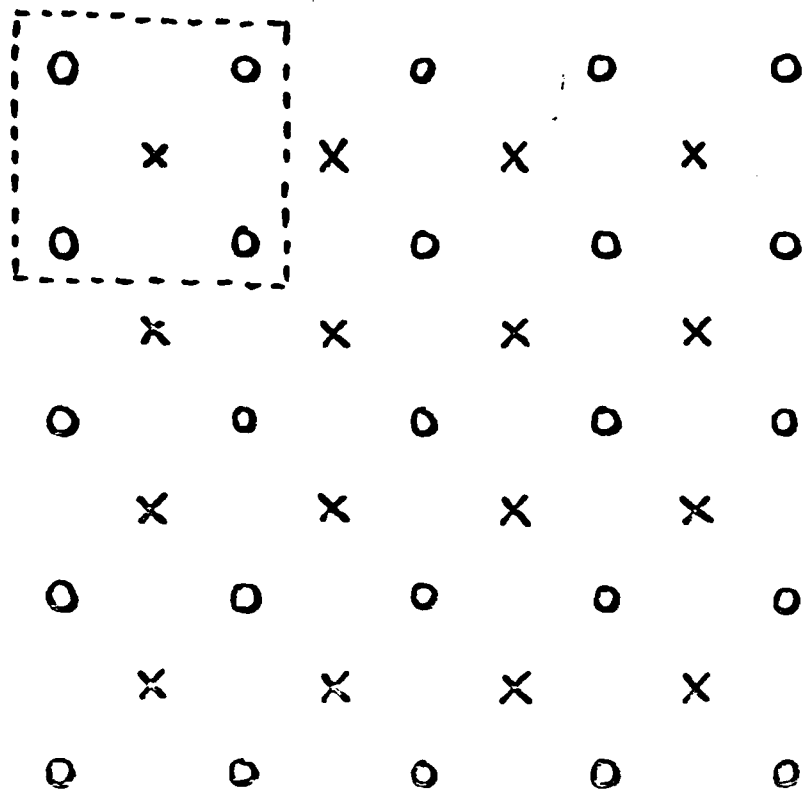


Fig 1

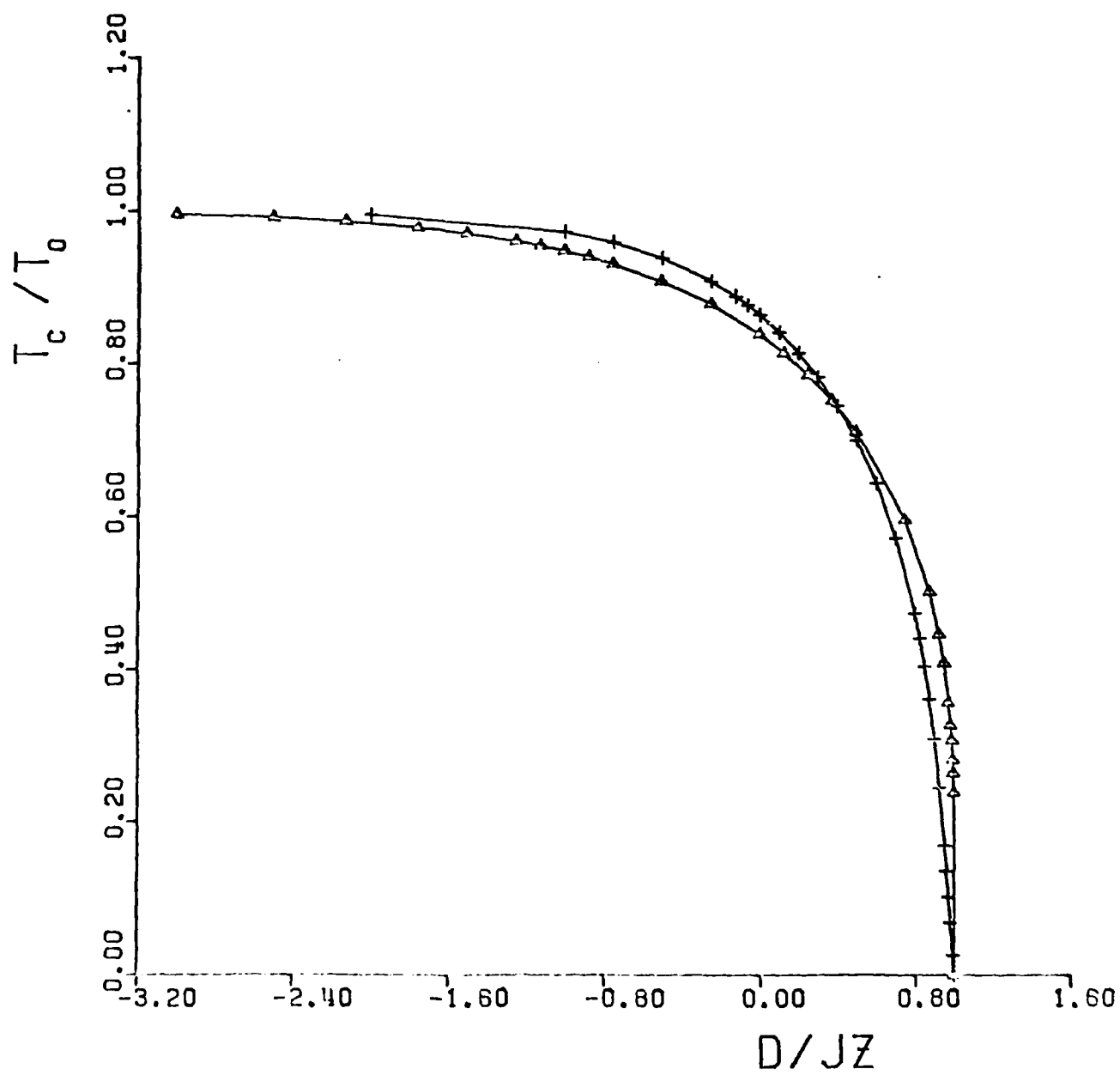


Fig 2

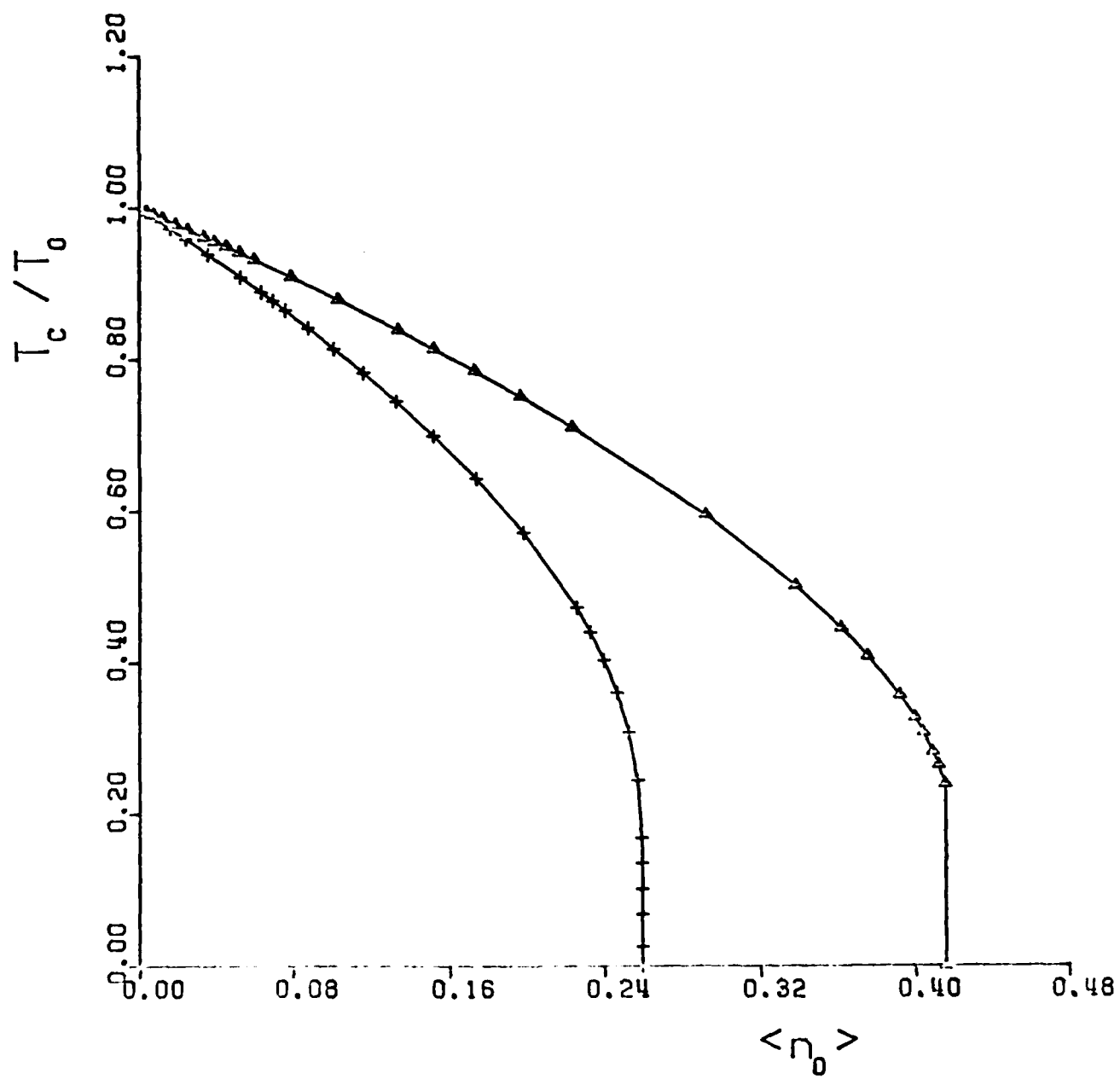


Fig 3

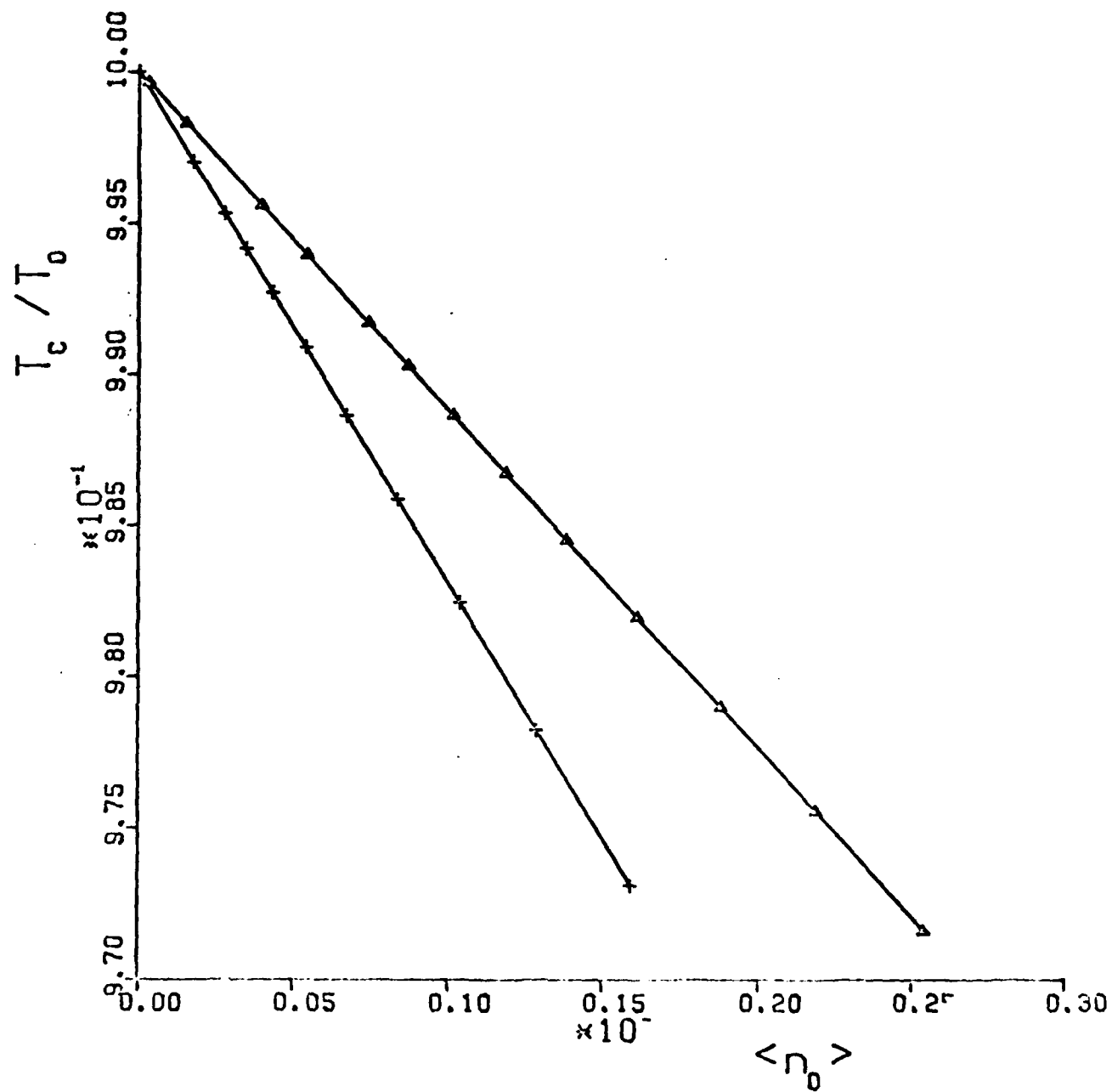


Fig 4



**DATA  
FILM**